STRUCTURE FILE UPDATES: 2 DEC 2002 HIGHEST RN 474876-19-2
DICTIONARY FILE UPDATES: 2 DEC 2002 HIGHEST RN 474876-19-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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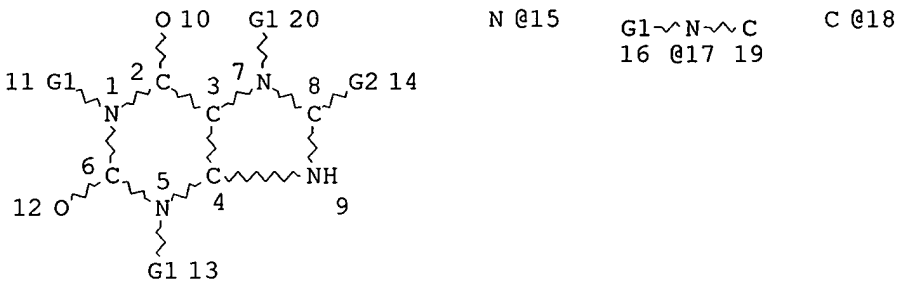
L1 STR



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VAR G2=15/17/18
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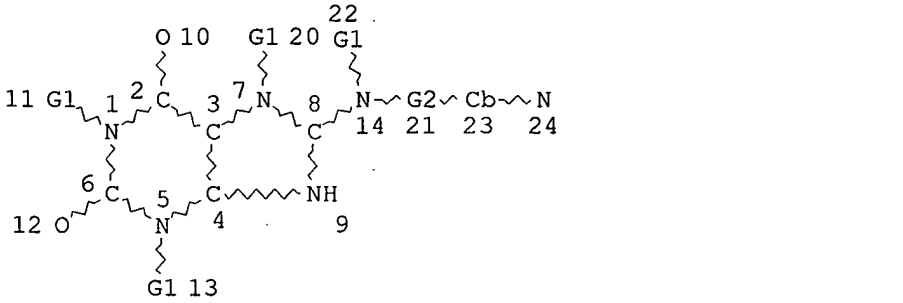
NSPEC IS R AT 15
NSPEC IS RC AT 18
NSPEC IS RC AT 19
CONNECT IS M1 RC AT 10
CONNECT IS M1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L3 5409 SEA FILE=REGISTRY SSS FUL L1
L24 STR



Searched by: Mary Hale 308-4258 CM-1 1E01

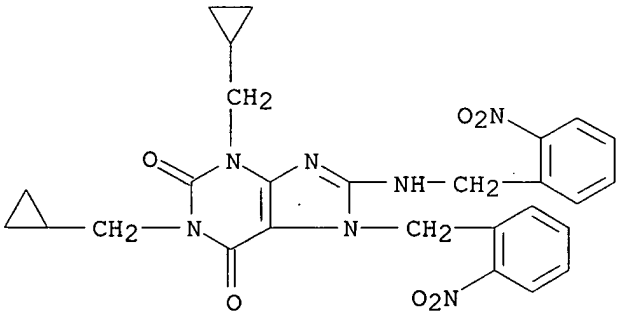
VAR G1=H/C
REP G2=(1-2) C
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 10
CONNECT IS M1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L25 7 SEA FILE=REGISTRY SUB=L3 SSS FUL L24

100.0% PROCESSED 514 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L25 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 143410-95-1 REGISTRY
CN 1H-Purine-2,6-dione, 1,3-bis(cyclopropylmethyl)-3,7-dihydro-7-[(2-nitrophenyl)methyl]-8-[[(2-nitrophenyl)methyl]amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H27 N7 O6
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 117:151010 7-alkyl-8-aminoxanthine and 7-alkyl-8-chloroxanthine derivatives, a method for their preparation and their use as phosphodiesterase inhibitor, antiallergic and for treatment of eosinophilia. Buckle, Derek Richard; Smith, David Glynn; Fenwick, Ashley Edward (Beecham Group PLC, UK). PCT Int. Appl. WO 9205175 A1 19920402, 54 pp. DESIGNATED STATES: W: AU, CA, JP, KR, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1991-GB1633 19910923. PRIORITY: GB 1990-20959 19900926.

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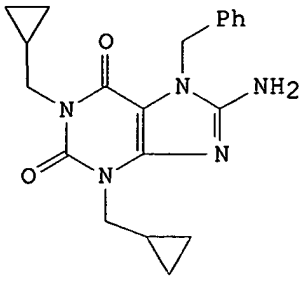
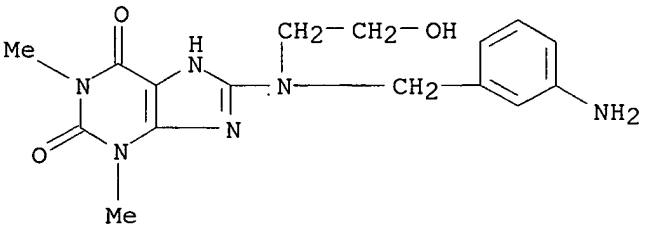
GI



I

AB Certain 7-alkylxanthine derivs. (7-alkyl-1H-purine-2,6-diones) are claimed. A process for their prepn. comprises the alkylation of a xanthine deriv. Pharmaceuticals contg. said compds. are claimed for the treatment of disorders assocd. with increased nos. of eosinophils and allergic disorders assocd. with atopy; the compds. are phosphodiesterase inhibitors. These compds. have potential use as inhibitors for tumor necrosis factor, HIV, AIDS, arthritis, and for the treatment of conditions assocd. with infection (no data). Treatment of 8-amino-1,3-bis(cyclopropylmethyl)xanthine with KOCMe3/DMF and benzyl bromide gave 8-amino-7-benzyl-1,3-bis(cyclopropylmethyl)xanthine (I) in 84% yield. I was active in the treatment of blood eosinophilia in rats and had activity as phosphodiesterase inhibitor.

L25 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 40171-63-9 REGISTRY
CN 1H-Purine-2,6-dione, 8-[[(3-aminophenyl)methyl](2-hydroxyethyl)amino]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H20 N6 O3
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

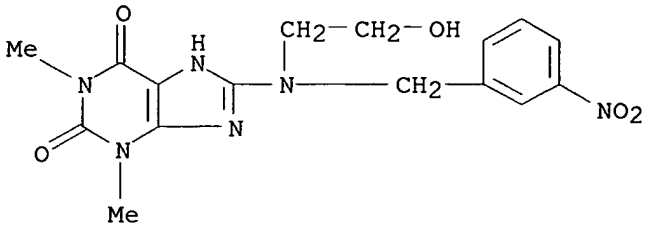
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 78:72181 8-Aminotheophylline derivatives. (Laboratoire Lebrun S. A.). Fr. Demande FR 2116302 19720818, 15 pp. (French). CODEN: FRXXBL. APPLICATION: FR 1970-43891 19701207.
GI For diagram(s), see printed CA Issue.
AB 8-Aminotheophyllines I (R = alkyl, aralkyl, hydroxyalkyl, chloroalkyl, aminoalkyl; R1 = alkyl, aralkyl, aminoalkyl; NRR1 = substituted

Searched by: Mary Hale 308-4258 CM-1 1E01

piperazino, piperidino, pyrrolidino) (52 compds.) were prepd. by treating 8-chlorotheophylline or 8-bromotheophylline with RR1NH. I displayed coronary dilator, diuretic, spasmolytic, and bronchodilator activities greater than that of theophylline, accompanied by lower toxicity.

L25 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 40171-62-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[(2-hydroxyethyl)[(3-nitrophenyl)methyl]amino]-1,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H18 N6 O5
LC STN Files: CA, CAPLUS, TOXCENTER



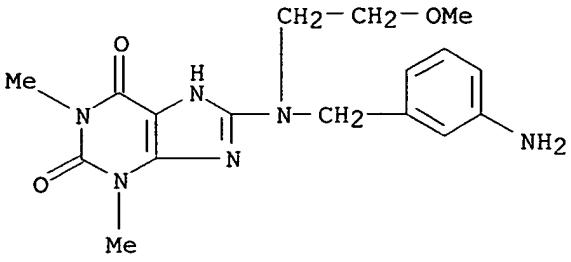
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 78:72181 8-Aminotheophylline derivatives. (Laboratoire Lebrun S. A.). Fr. Demande FR 2116302 19720818, 15 pp. (French). CODEN: FRXXBL. APPLICATION: FR 1970-43891 19701207.
GI For diagram(s), see printed CA Issue.
AB 8-Aminotheophyllines I (R = alkyl, aralkyl, hydroxyalkyl, chloroalkyl, aminoalkyl; R1 = alkyl, aralkyl, aminoalkyl; NRR1 = substituted piperazino, piperidino, pyrrolidino) (52 compds.) were prepd. by treating 8-chlorotheophylline or 8-bromotheophylline with RR1NH. I displayed coronary dilator, diuretic, spasmolytic, and bronchodilator activities greater than that of theophylline, accompanied by lower toxicity.

L25 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 36750-31-9 REGISTRY
CN 1H-Purine-2,6-dione, 8-[[(3-aminophenyl)methyl](2-methoxyethyl)amino]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H22 N6 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

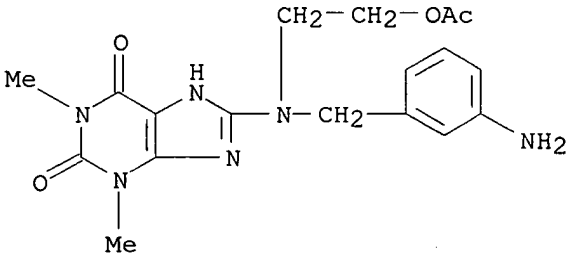
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 77:101678 8-Aminotheophyllines. Laboratoire le Bruns S. A. Ger. Offen. DE 2160382 19720622, 26 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1971-2160382 19711206.

GI For diagram(s), see printed CA Issue.

AB About 110 title compds. [I, n = 2 or 3; R = H, Me, Et, (CH2)mOMe with m = 2 or 3, (CH2)m-OEt, (CH2)mOH, CH2CH(OH)Me, CH2CH(OH)CH2OH, CH2CH2OPh, CH2CH2OAc, 3,4-(OCH2O)C6H3CH2, CH2C6H5-nRn3 with R3 = H, p-Me, OMe, (OMe)2, 3,4,5-(OMe)3, p-Cl, Cl2, m-NO2, m-NH2, or p-OAc; R1 = Me, Et, CH2CH2OH, Ph, CHO, Ac, COEt, or Bz] were prepd. by reaction of 8-chlorotheophylline with amines RNH(CH2)nOR4 (R4 = H, Me, Et, CH2CH2OH, or Ph) and optional acylation. I were used as analgesics, antitussives, diuretics, antiinflammatants, spasmolytics, coronary dilators, and bronchi dilators. The spasmolytic activity (ED50 in mg/kg) of I [n = 2, R = 3,4-(OMe)2C6H3CH2, R1 = Ac] (II) in rabbit was 300, compared to 100 of papaverine, the coronary dilation by II in rabbit was 100, equiv. to theophylline, and the antitussive effect of II in guinea pigs was 110, equiv. to codeine.

L25 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 36746-46-0 REGISTRY
CN 1H-Purine-2,6-dione, 8-[[2-(acetyloxy)ethyl][(3-aminophenyl)methyl]amino]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O4
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

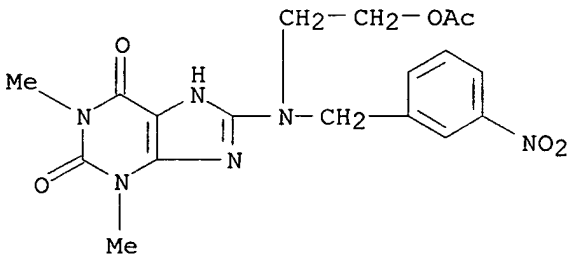
1 REFERENCES IN FILE CA (1962 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 77:101678 8-Aminotheophyllines. Laboratoire le Bruns S. A. Ger. Offen. DE 2160382 19720622, 26 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1971-2160382 19711206.
GI For diagram(s), see printed CA Issue.
AB About 110 title compds. [I, n = 2 or 3; R = H, Me, Et, (CH2)mOMe with m = 2 or 3, (CH2)m-OEt, (CH2)mOH, CH2CH(OH)Me, CH2CH(OH)CH2OH, CH2CH2OPh, CH2CH2OAc, 3,4-(OCH2O)C6H3CH2, CH2C6H5-nRn3 with R3 = H, p-Me, OMe, (OMe)2, 3,4,5-(OMe)3, p-Cl, Cl2, m-NO2, m-NH2, or p-OAc; R1 = Me, Et, CH2CH2OH, Ph, CHO, Ac, COEt, or Bz] were prepd. by reaction of 8-chlorotheophylline with amines RNH(CH2)nOR4 (R4 = H, Me, Et, CH2CH2OH, or Ph) and optional acylation. I were used as analgesics, antitussives, diuretics, antiinflammatants, spasmolytics, coronary dilators, and bronchi dilators. The spasmolytic activity (ED50 in mg/kg) of I [n = 2, R = 3,4-(OMe)2C6H3CH2, R1 = Ac] (II) in rabbit was 300, compared to 100 of papaverine, the coronary dilation by II in rabbit was 100, equiv. to theophylline, and the antitussive effect of II in guinea pigs was 110, equiv. to codeine.

L25 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 36746-45-9 REGISTRY
CN 1H-Purine-2,6-dione, 8-[[2-(acetyloxy)ethyl][(3-nitrophenyl)methyl]amino]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H20 N6 O6
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

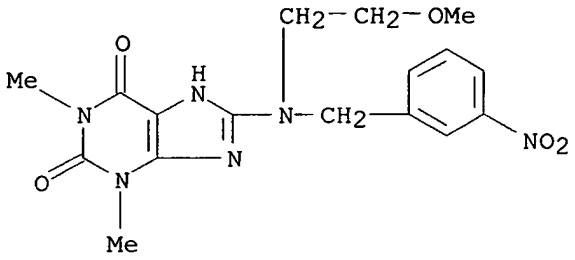
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 77:101678 8-Aminotheophyllines. Laboratoire le Bruns S. A. Ger. Offen. DE 2160382 19720622, 26 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1971-2160382 19711206.
GI For diagram(s), see printed CA Issue.
AB About 110 title compds. [I, n = 2 or 3; R = H, Me, Et, (CH2)mOMe with m = 2 or 3, (CH2)m-OEt, (CH2)mOH, CH2CH(OH)Me, CH2CH(OH)CH2OH, CH2CH2OPh, CH2CH2OAc, 3,4-(OCH2O)C6H3CH2, CH2C6H5-nRn3 with R3 = H, p-Me, OMe, (OMe)2, 3,4,5-(OMe)3, p-Cl, Cl2, m-NO2, m-NH2, or p-OAc; R1 = Me, Et, CH2CH2OH, Ph, CHO, Ac, COEt, or Bz] were prepd. by reaction of 8-chlorotheophylline with amines RNH(CH2)nOR4 (R4 = H, Me, Et, CH2CH2OH, or Ph) and optional acylation. I were used as analgesics, antitussives, diuretics, antiinflammatants, spasmolytics, coronary dilators, and bronchi dilators. The spasmolytic activity (ED50 in mg/kg) of I [n = 2, R = 3,4-(OMe)2C6H3CH2, R1 = Ac] (II) in rabbit was 300, compared to 100 of

Searched by: Mary Hale 308-4258 CM-1 1E01

papaverine, the coronary dilation by II in rabbit was 100, equiv. to theophylline, and the antitussive effect of II in guinea pigs was 110, equiv. to codeine.

L25 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2002 ACS
RN 36740-68-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[(2-methoxyethyl)[(3-nitrophenyl)methyl]amino]-1,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H20 N6 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 77:101678 8-Aminotheophyllines. Laboratoire le Bruns S. A. Ger. Offen. DE 2160382 19720622, 26 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1971-2160382 19711206.
GI For diagram(s), see printed CA Issue.
AB About 110 title compds. [I, n = 2 or 3; R = H, Me, Et, (CH2)mOMe with m = 2 or 3, (CH2)m-OEt, (CH2)mOH, CH2CH(OH)Me, CH2CH(OH)CH2OH, CH2CH2OPh, CH2CH2OAc, 3,4-(OCH2O)C6H3CH2, CH2C6H5-nRn3 with R3 = H, p-Me, OMe, (OMe)2, 3,4,5-(OMe)3, p-Cl, Cl2, m-NO2, m-NH2, or p-OAc; R1 = Me, Et, CH2CH2OH, Ph, CHO, Ac, COEt, or Bz] were prepd. by reaction of 8-chlorotheophylline with amines RNH(CH2)nOR4 (R4 = H, Me, Et, CH2CH2OH, or Ph) and optional acylation. I were used as analgesics, antitussives, diuretics, antiinflammatants, spasmolytics, coronary dilators, and bronchi dilators. The spasmolytic activity (ED50 in mg/kg) of I [n = 2, R = 3,4-(OMe)2C6H3CH2, R1 = Ac] (II) in rabbit was 300, compared to 100 of papaverine, the coronary dilation by II in rabbit was 100, equiv. to theophylline, and the antitussive effect of II in guinea pigs was 110, equiv. to codeine.

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Searched by: Mary Hale 308-4258 CM-1 1E01